



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:27 AM UTC

PDB ID : 5XWV / pdb_00005xwv
Title : Substrate-bound Structure of a Ketoreductase from the Second Module of the amphotericin Polyketide Synthases
Authors : Liu, C.; Zheng, J.
Deposited on : 2017-06-30
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

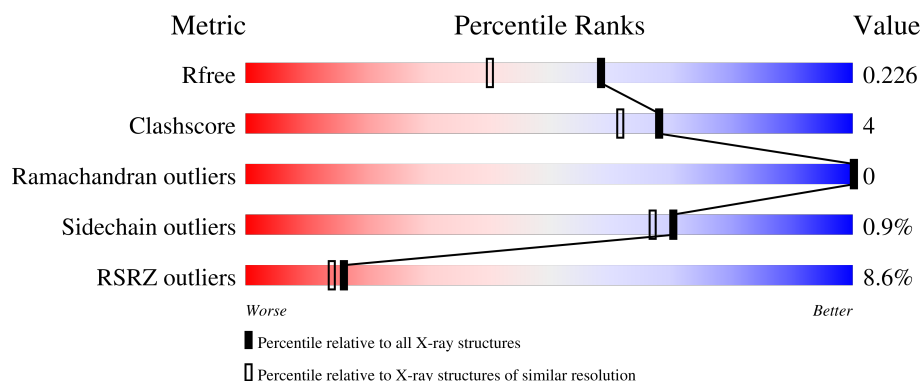
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	10% 89% 8%
1	B	496	6% 90% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7352 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AmphB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3469	2165	636	659	9			
1	B	477	Total	C	N	O	S	0	0	0
			3469	2165	636	659	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q93NW7
A	-19	GLY	-	expression tag	UNP Q93NW7
A	-18	SER	-	expression tag	UNP Q93NW7
A	-17	SER	-	expression tag	UNP Q93NW7
A	-16	HIS	-	expression tag	UNP Q93NW7
A	-15	HIS	-	expression tag	UNP Q93NW7
A	-14	HIS	-	expression tag	UNP Q93NW7
A	-13	HIS	-	expression tag	UNP Q93NW7
A	-12	HIS	-	expression tag	UNP Q93NW7
A	-11	HIS	-	expression tag	UNP Q93NW7
A	-10	SER	-	expression tag	UNP Q93NW7
A	-9	SER	-	expression tag	UNP Q93NW7
A	-8	GLY	-	expression tag	UNP Q93NW7
A	-7	LEU	-	expression tag	UNP Q93NW7
A	-6	VAL	-	expression tag	UNP Q93NW7
A	-5	PRO	-	expression tag	UNP Q93NW7
A	-4	ARG	-	expression tag	UNP Q93NW7
A	-3	GLY	-	expression tag	UNP Q93NW7
A	-2	SER	-	expression tag	UNP Q93NW7
A	-1	HIS	-	expression tag	UNP Q93NW7
A	0	MET	-	expression tag	UNP Q93NW7
B	-20	MET	-	expression tag	UNP Q93NW7
B	-19	GLY	-	expression tag	UNP Q93NW7
B	-18	SER	-	expression tag	UNP Q93NW7
B	-17	SER	-	expression tag	UNP Q93NW7

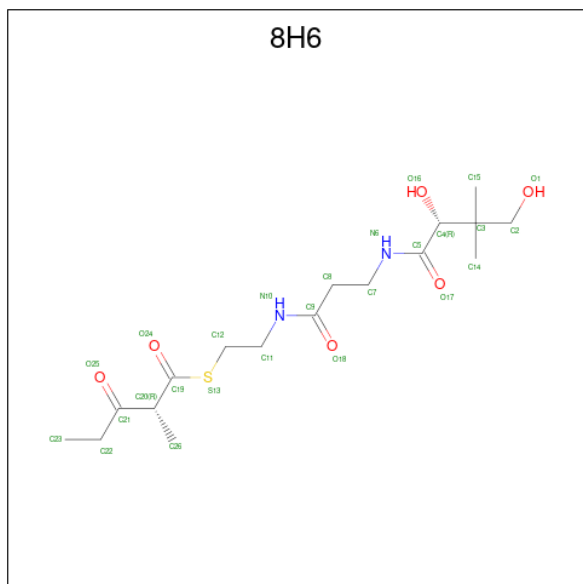
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q93NW7
B	-15	HIS	-	expression tag	UNP Q93NW7
B	-14	HIS	-	expression tag	UNP Q93NW7
B	-13	HIS	-	expression tag	UNP Q93NW7
B	-12	HIS	-	expression tag	UNP Q93NW7
B	-11	HIS	-	expression tag	UNP Q93NW7
B	-10	SER	-	expression tag	UNP Q93NW7
B	-9	SER	-	expression tag	UNP Q93NW7
B	-8	GLY	-	expression tag	UNP Q93NW7
B	-7	LEU	-	expression tag	UNP Q93NW7
B	-6	VAL	-	expression tag	UNP Q93NW7
B	-5	PRO	-	expression tag	UNP Q93NW7
B	-4	ARG	-	expression tag	UNP Q93NW7
B	-3	GLY	-	expression tag	UNP Q93NW7
B	-2	SER	-	expression tag	UNP Q93NW7
B	-1	HIS	-	expression tag	UNP Q93NW7
B	0	MET	-	expression tag	UNP Q93NW7

- # NDP
-
- The chemical structure of NDP (Nucleoside Diphosphate) is shown. It consists of a pyrimidine base (labeled N1A, N1B, C3A, C3B, C4A, C4B, C5A, C5B, C6A, C6B) attached to a ribose sugar (labeled C1', C2', C3', C4', C5'). The ribose sugar is further attached to a diphosphate group (labeled O1P, O2P, O3P, O4P, O5P, O6P, O7P, O8P, O9P, O10P, O11P, O12P, O13P, O14P, O15P, O16P, O17P, O18P, O19P, O20P, O21P, O22P, O23P, O24P, O25P, O26P, O27P, O28P, O29P, O30P, O31P, O32P, O33P, O34P, O35P, O36P, O37P, O38P, O39P, O40P, O41P, O42P, O43P, O44P, O45P, O46P, O47P, O48P, O49P, O50P, O51P, O52P, O53P, O54P, O55P, O56P, O57P, O58P, O59P, O60P, O61P, O62P, O63P, O64P, O65P, O66P, O67P, O68P, O69P, O70P, O71P, O72P, O73P, O74P, O75P, O76P, O77P, O78P, O79P, O80P, O81P, O82P, O83P, O84P, O85P, O86P, O87P, O88P, O89P, O90P, O91P, O92P, O93P, O94P, O95P, O96P, O97P, O98P, O99P, O100P, O101P, O102P, O103P, O104P, O105P, O106P, O107P, O108P, O109P, O110P, O111P, O112P, O113P, O114P, O115P, O116P, O117P, O118P, O119P, O120P, O121P, O122P, O123P, O124P, O125P, O126P, O127P, O128P, O129P, O130P, O131P, O132P, O133P, O134P, O135P, O136P, O137P, O138P, O139P, O140P, O141P, O142P, O143P, O144P, O145P, O146P, O147P, O148P, O149P, O150P, O151P, O152P, O153P, O154P, O155P, O156P, O157P, O158P, O159P, O160P, O161P, O162P, O163P, O164P, O165P, O166P, O167P, O168P, O169P, O170P, O171P, O172P, O173P, O174P, O175P, O176P, O177P, O178P, O179P, O180P, O181P, O182P, O183P, O184P, O185P, O186P, O187P, O188P, O189P, O190P, O191P, O192P, O193P, O194P, O195P, O196P, O197P, O198P, O199P, O200P, O201P, O202P, O203P, O204P, O205P, O206P, O207P, O208P, O209P, O210P, O211P, O212P, O213P, O214P, O215P, O216P, O217P, O218P, O219P, O220P, O221P, O222P, O223P, O224P, O225P, O226P, O227P, O228P, O229P, O230P, O231P, O232P, O233P, O234P, O235P, O236P, O237P, O238P, O239P, O240P, O241P, O242P, O243P, O244P, O245P, O246P, O247P, O248P, O249P, O250P, O251P, O252P, O253P, O254P, O255P, O256P, O257P, O258P, O259P, O260P, O261P, O262P, O263P, O264P, O265P, O266P, O267P, O268P, O269P, O270P, O271P, O272P, O273P, O274P, O275P, O276P, O277P, O278P, O279P, O280P, O281P, O282P, O283P, O284P, O285P, O286P, O287P, O288P, O289P, O290P, O291P, O292P, O293P, O294P, O295P, O296P, O297P, O298P, O299P, O300P, O301P, O302P, O303P, O304P, O305P, O306P, O307P, O308P, O309P, O310P, O311P, O312P, O313P, O314P, O315P, O316P, O317P, O318P, O319P, O320P, O321P, O322P, O323P, O324P, O325P, O326P, O327P, O328P, O329P, O330P, O331P, O332P, O333P, O334P, O335P, O336P, O337P, O338P, O339P, O340P, O341P, O342P, O343P, O344P, O345P, O346P, O347P, O348P, O349P, O350P, O351P, O352P, O353P, O354P, O355P, O356P, O357P, O358P, O359P, O360P, O361P, O362P, O363P, O364P, O365P, O366P, O367P, O368P, O369P, O370P, O371P, O372P, O373P, O374P, O375P, O376P, O377P, O378P, O379P, O380P, O381P, O382P, O383P, O384P, O385P, O386P, O387P, O388P, O389P, O390P, O391P, O392P, O393P, O394P, O395P, O396P, O397P, O398P, O399P, O400P, O401P, O402P, O403P, O404P, O405P, O406P, O407P, O408P, O409P, O410P, O411P, O412P, O413P, O414P, O415P, O416P, O417P, O418P, O419P, O420P, O421P, O422P, O423P, O424P, O425P, O426P, O427P, O428P, O429P, O430P, O431P, O432P, O433P, O434P, O435P, O436P, O437P, O438P, O439P, O440P, O441P, O442P, O443P, O444P, O445P, O446P, O447P, O448P, O449P, O450P, O451P, O452P, O453P, O454P, O455P, O456P, O457P, O458P, O459P, O460P, O461P, O462P, O463P, O464P, O465P, O466P, O467P, O468P, O469P, O470P, O471P, O472P, O473P, O474P, O475P, O476P, O477P, O478P, O479P, O480P, O481P, O482P, O483P, O484P, O485P, O486P, O487P, O488P, O489P, O490P, O491P, O492P, O493P, O494P, O495P, O496P, O497P, O498P, O499P, O500P, O501P, O502P, O503P, O504P, O505P, O506P, O507P, O508P, O509P, O510P, O511P, O512P, O513P, O514P, O515P, O516P, O517P, O518P, O519P, O520P, O521P, O522P, O523P, O524P, O525P, O526P, O527P, O528P, O529P, O530P, O531P, O532P, O533P, O534P, O535P, O536P, O537P, O538P, O539P, O540P, O541P, O542P, O543P, O544P, O545P, O546P, O547P, O548P, O549P, O550P, O551P, O552P, O553P, O554P, O555P, O556P, O557P, O558P, O559P, O560P, O561P, O562P, O563P, O564P, O565P, O566P, O567P, O568P, O569P, O570P, O571P, O572P, O573P, O574P, O575P, O576P, O577P, O578P, O579P, O580P, O581P, O582P, O583P, O584P, O585P, O586P, O587P, O588P, O589P, O590P, O591P, O592P, O593P, O594P, O595P, O596P, O597P, O598P, O599P, O600P, O601P, O602P, O603P, O604P, O605P, O606P, O607P, O608P, O609P, O610P, O611P, O612P, O613P, O614P, O615P, O616P, O617P, O618P, O619P, O620P, O621P, O622P, O623P, O624P, O625P, O626P, O627P, O628P, O629P, O630P, O631P, O632P, O633P, O634P, O635P, O636P, O637P, O638P, O639P, O640P, O641P, O642P, O643P, O644P, O645P, O646P, O647P, O648P, O649P, O650P, O651P, O652P, O653P, O654P, O655P, O656P, O657P, O658P, O659P, O660P, O661P, O662P, O663P, O664P, O665P, O666P, O667P, O668P, O669P, O670P, O671P, O672P, O673P, O674P, O675P

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is S-[2-[3-[[[(2R)-3,3-dimethyl-2,4-bis(oxidanyl)butanoyl]amino]propanoyl amino]ethyl] (2R)-2-methyl-3-oxidanylidene-pentanethioate (CCD ID: 8H6) (formula: C₁₇H₃₀N₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	17	2	6	1		
3	B	1	Total	C	N	O	S	0	0
			26	17	2	6	1		

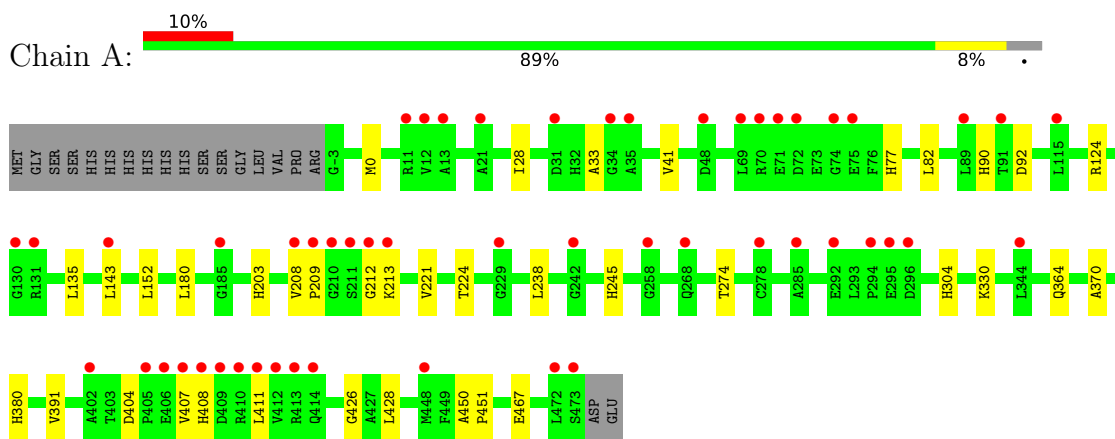
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	0
			128	128		
4	B	138	Total	O	0	0
			138	138		

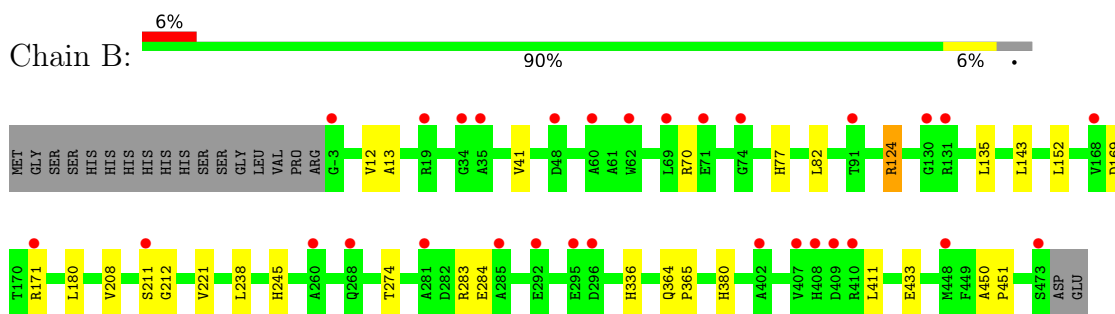
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: AmphB



• Molecule 1: AmphB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.32Å 63.56Å 71.89Å 73.09° 67.20° 89.76°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-1.80) 91.5 (50.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.180 , 0.217 0.190 , 0.226	Depositor DCC
R_{free} test set	4164 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.157 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7352	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 8H6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3539	0.64	0/4834
1	B	0.63	0/3539	0.62	0/4834
All	All	0.62	0/7078	0.63	0/9668

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3469	0	3429	26	0
1	B	3469	0	3429	22	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
3	A	26	0	0	6	0
3	B	26	0	0	5	0
4	A	128	0	0	2	0
4	B	138	0	0	1	0
All	All	7352	0	6910	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG23	1:B:211:SER:OG	1.68	0.92
1:A:404:ASP:O	1:A:407:VAL:HG12	1.80	0.82
1:A:90:HIS:HD2	1:A:92:ASP:H	1.34	0.73
1:A:364:GLN:NE2	3:A:502:8H6:S13	2.61	0.64
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.82	0.63
1:B:77:HIS:HE1	1:B:180:LEU:O	1.83	0.62
1:A:203:HIS:HD2	4:A:643:HOH:O	1.83	0.61
1:B:208:VAL:CG2	1:B:211:SER:OG	2.46	0.61
1:B:221:VAL:HG11	1:B:238:LEU:HD13	1.82	0.61
1:B:152:LEU:HD22	3:B:502:8H6:C14	2.31	0.60
1:A:77:HIS:HE1	1:A:180:LEU:O	1.85	0.60
1:B:283:ARG:HH21	1:B:336:HIS:HD2	1.48	0.60
1:A:203:HIS:HE1	1:A:467:GLU:OE2	1.85	0.60
1:B:208:VAL:HG23	1:B:211:SER:CB	2.32	0.58
1:A:90:HIS:CD2	1:A:92:ASP:H	2.18	0.57
1:A:450:ALA:HB3	1:A:451:PRO:HD3	1.86	0.56
1:A:224:THR:OG1	1:A:304:HIS:HD2	1.88	0.55
1:B:450:ALA:HB3	1:B:451:PRO:HD3	1.89	0.53
1:A:224:THR:OG1	1:A:304:HIS:CD2	2.62	0.53
1:B:124:ARG:O	1:B:124:ARG:HG3	2.09	0.53
1:B:411:LEU:CD2	3:B:502:8H6:C11	2.87	0.52
3:B:502:8H6:C23	3:B:502:8H6:C26	2.87	0.52
1:A:152:LEU:HD22	3:A:502:8H6:C14	2.39	0.52
1:A:407:VAL:HG13	1:A:408:HIS:N	2.26	0.51
3:A:502:8H6:C23	3:A:502:8H6:C26	2.88	0.51
1:A:411:LEU:CD2	3:A:502:8H6:C11	2.88	0.51
3:A:502:8H6:C15	4:A:720:HOH:O	2.58	0.50
1:B:171:ARG:CG	4:B:671:HOH:O	2.59	0.50
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.96	0.49
1:B:364:GLN:OE1	3:B:502:8H6:S13	2.71	0.48
1:A:245:HIS:CE1	1:A:274:THR:OG1	2.64	0.48
1:B:208:VAL:HG23	1:B:208:VAL:O	2.15	0.47
1:B:169:ASP:OD1	1:B:171:ARG:HG2	2.15	0.47
1:A:209:PRO:HD2	1:B:13:ALA:HB2	1.96	0.46
1:B:135:LEU:O	1:B:380:HIS:HD2	1.99	0.45
1:B:41:VAL:HG11	1:B:82:LEU:HD21	1.97	0.45
3:B:502:8H6:O18	3:B:502:8H6:C12	2.60	0.45
1:B:283:ARG:HH21	1:B:336:HIS:CD2	2.31	0.45
1:A:407:VAL:CG1	1:A:408:HIS:N	2.80	0.45
1:A:0:MET:SD	1:A:426:GLY:HA3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HG21	1:A:428:LEU:HD13	1.99	0.44
1:B:212:GLY:HA3	1:B:433:GLU:OE2	2.18	0.44
1:A:208:VAL:HG13	1:B:12:VAL:O	2.19	0.43
3:A:502:8H6:O18	3:A:502:8H6:C12	2.67	0.43
1:A:221:VAL:HG11	1:A:238:LEU:HD13	2.01	0.43
1:A:135:LEU:O	1:A:380:HIS:HD2	2.03	0.41
1:A:41:VAL:HG11	1:A:82:LEU:HD21	2.03	0.41
1:B:364:GLN:N	1:B:365:PRO:CD	2.83	0.41
1:A:212:GLY:O	1:A:213:LYS:HB2	2.21	0.41
1:A:330:LYS:HG3	1:A:370:ALA:HB1	2.03	0.40
1:A:28:ILE:CG2	1:A:33:ALA:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	475/496 (96%)	460 (97%)	15 (3%)	0	100	100
1	B	475/496 (96%)	463 (98%)	12 (2%)	0	100	100
All	All	950/992 (96%)	923 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/351 (95%)	332 (99%)	2 (1%)	78	77
1	B	334/351 (95%)	330 (99%)	4 (1%)	63	57
All	All	668/702 (95%)	662 (99%)	6 (1%)	70	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	143	LEU
1	B	70	ARG
1	B	124	ARG
1	B	143	LEU
1	B	284	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	32	HIS
1	A	65	GLN
1	A	68	GLN
1	A	77	HIS
1	A	90	HIS
1	A	102	GLN
1	A	203	HIS
1	A	245	HIS
1	A	304	HIS
1	A	380	HIS
1	B	65	GLN
1	B	68	GLN
1	B	77	HIS
1	B	245	HIS
1	B	336	HIS
1	B	364	GLN
1	B	380	HIS
1	B	423	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	8H6	A	502	-	21,25,25	1.45	2 (9%)	26,33,33	2.43	10 (38%)
2	NDP	B	501	-	51,52,52	1.29	7 (13%)	71,80,80	1.53	10 (14%)
2	NDP	A	501	-	51,52,52	1.24	4 (7%)	71,80,80	1.56	12 (16%)
3	8H6	B	502	-	21,25,25	1.43	2 (9%)	26,33,33	2.21	10 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8H6	A	502	-	-	15/36/36/36	-
2	NDP	B	501	-	-	5/34/77/77	0/5/5/5
2	NDP	A	501	-	-	7/34/77/77	0/5/5/5
3	8H6	B	502	-	-	14/36/36/36	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	8H6	C9-N10	-3.87	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NDP	C5A-C4A	3.86	1.46	1.39
2	B	501	NDP	PA-O3	3.80	1.63	1.59
3	A	502	8H6	C9-N10	-3.72	1.24	1.33
2	A	501	NDP	C4A-N9A	-3.50	1.30	1.37
2	B	501	NDP	C5A-C4A	3.49	1.45	1.39
3	A	502	8H6	C19-S13	-3.33	1.64	1.75
3	B	502	8H6	C19-S13	-3.05	1.64	1.75
2	A	501	NDP	C5A-N7A	-2.95	1.33	1.39
2	B	501	NDP	PN-O3	2.94	1.62	1.59
2	B	501	NDP	C4A-N9A	-2.49	1.32	1.37
2	A	501	NDP	P2B-O2B	2.31	1.63	1.59
2	B	501	NDP	C5A-N7A	-2.16	1.35	1.39
2	B	501	NDP	C8A-N7A	2.05	1.35	1.31
2	B	501	NDP	P2B-O2B	2.00	1.63	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	8H6	C7-N6-C5	6.96	135.05	122.55
3	B	502	8H6	C7-N6-C5	6.44	134.11	122.55
3	A	502	8H6	C4-C5-N6	4.79	125.57	116.48
2	B	501	NDP	C5A-C4A-N3A	-4.65	120.31	126.72
2	A	501	NDP	C5A-C4A-N3A	-4.58	120.41	126.72
2	B	501	NDP	N3A-C2A-N1A	-4.21	122.20	128.58
3	B	502	8H6	C4-C5-N6	4.18	124.41	116.48
2	A	501	NDP	N3A-C2A-N1A	-4.09	122.39	128.58
3	A	502	8H6	C23-C22-C21	-3.81	105.62	115.02
2	B	501	NDP	C4A-N9A-C8A	3.70	109.63	105.74
2	A	501	NDP	N3A-C4A-N9A	3.52	133.16	127.17
2	A	501	NDP	C4A-C5A-N7A	-3.39	106.70	110.58
2	B	501	NDP	N3A-C4A-N9A	3.30	132.77	127.17
3	A	502	8H6	C12-S13-C19	3.24	111.02	101.73
2	A	501	NDP	C2A-N3A-C4A	3.19	119.62	111.83
2	A	501	NDP	C4A-N9A-C8A	3.14	109.04	105.74
3	B	502	8H6	C12-S13-C19	3.14	110.73	101.73
2	B	501	NDP	C2A-N3A-C4A	3.13	119.47	111.83
2	B	501	NDP	N9A-C8A-N7A	-3.05	109.61	113.94
2	B	501	NDP	C4A-C5A-N7A	-2.95	107.20	110.58
2	A	501	NDP	C2A-N1A-C6A	2.93	123.54	118.73
2	A	501	NDP	N9A-C8A-N7A	-2.80	109.97	113.94
3	A	502	8H6	O17-C5-N6	-2.77	117.12	122.98
2	A	501	NDP	O2B-P2B-O1X	-2.64	99.94	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	8H6	C7-C8-C9	2.62	116.76	112.39
2	A	501	NDP	C5A-N7A-C8A	2.60	107.54	103.45
2	A	501	NDP	C6N-N1N-C2N	2.52	122.02	119.32
2	B	501	NDP	O2B-P2B-O1X	-2.51	100.38	109.33
3	A	502	8H6	C12-C11-N10	-2.50	107.19	112.41
3	B	502	8H6	C23-C22-C21	-2.50	108.87	115.02
2	B	501	NDP	C5A-N7A-C8A	2.50	107.37	103.45
2	B	501	NDP	C2A-N1A-C6A	2.48	122.81	118.73
3	B	502	8H6	O17-C5-N6	-2.44	117.82	122.98
3	B	502	8H6	O18-C9-N10	-2.42	118.28	123.03
3	B	502	8H6	C12-C11-N10	-2.41	107.37	112.41
3	A	502	8H6	O18-C9-N10	-2.40	118.32	123.03
2	A	501	NDP	C6A-C5A-N7A	2.35	136.62	132.09
3	A	502	8H6	C15-C3-C2	-2.35	103.92	108.77
3	B	502	8H6	C15-C3-C2	-2.29	104.05	108.77
3	B	502	8H6	O24-C19-S13	-2.15	120.91	123.80
3	B	502	8H6	C15-C3-C4	2.13	112.39	108.77
3	A	502	8H6	C8-C7-N6	-2.07	107.60	112.00

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5D-O5D-PN-O3
2	A	501	NDP	C5D-O5D-PN-O2N
2	B	501	NDP	C5D-O5D-PN-O3
2	B	501	NDP	C5D-O5D-PN-O2N
3	A	502	8H6	O17-C5-N6-C7
3	A	502	8H6	C4-C5-N6-C7
3	A	502	8H6	C15-C3-C4-C5
3	A	502	8H6	C2-C3-C4-C5
3	A	502	8H6	C14-C3-C4-C5
3	A	502	8H6	C15-C3-C4-O16
3	A	502	8H6	C2-C3-C4-O16
3	A	502	8H6	C14-C3-C4-O16
3	A	502	8H6	C12-C11-N10-C9
3	A	502	8H6	N10-C11-C12-S13
3	A	502	8H6	C20-C21-C22-C23
3	A	502	8H6	O25-C21-C22-C23
3	B	502	8H6	O17-C5-N6-C7
3	B	502	8H6	C4-C5-N6-C7
3	B	502	8H6	C15-C3-C4-C5

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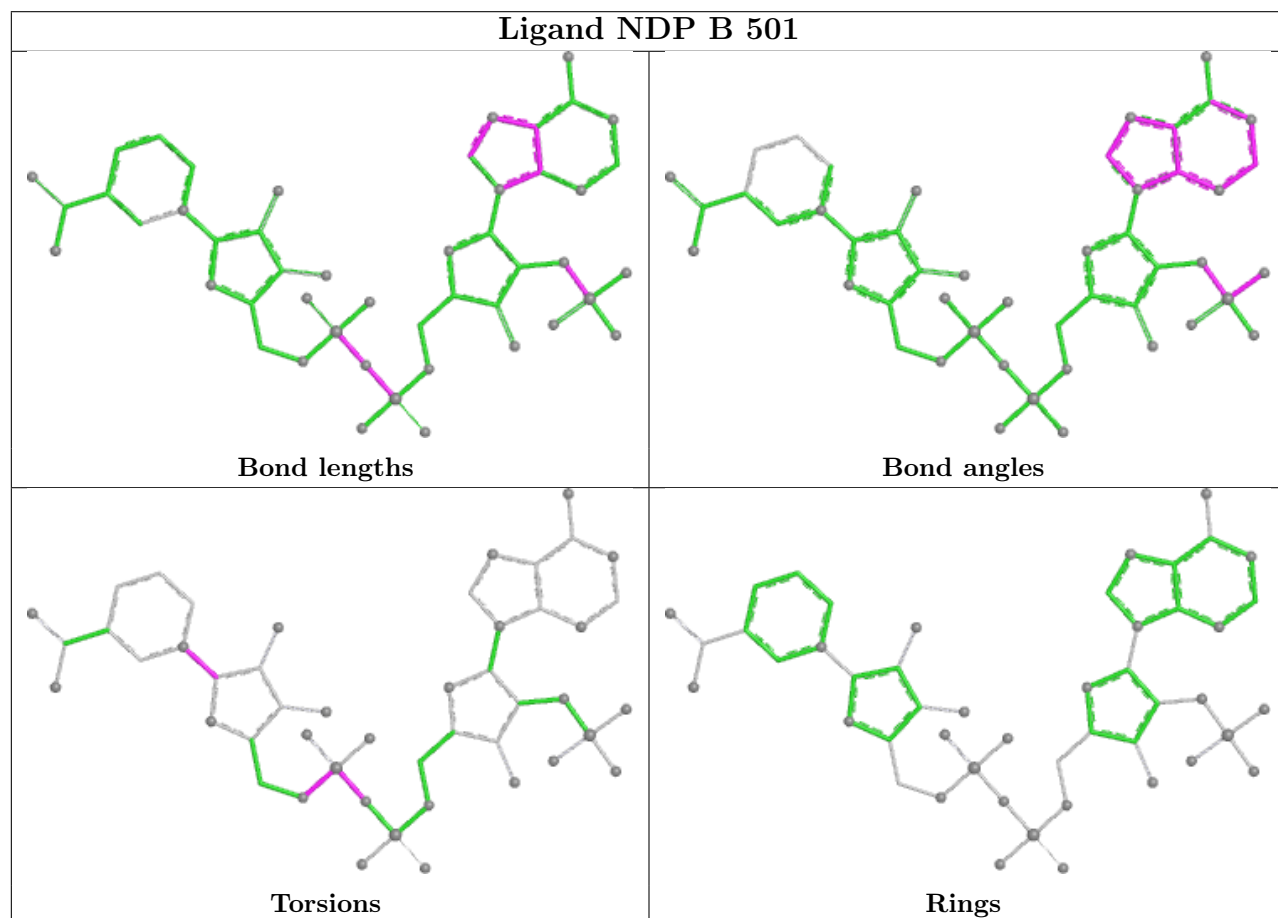
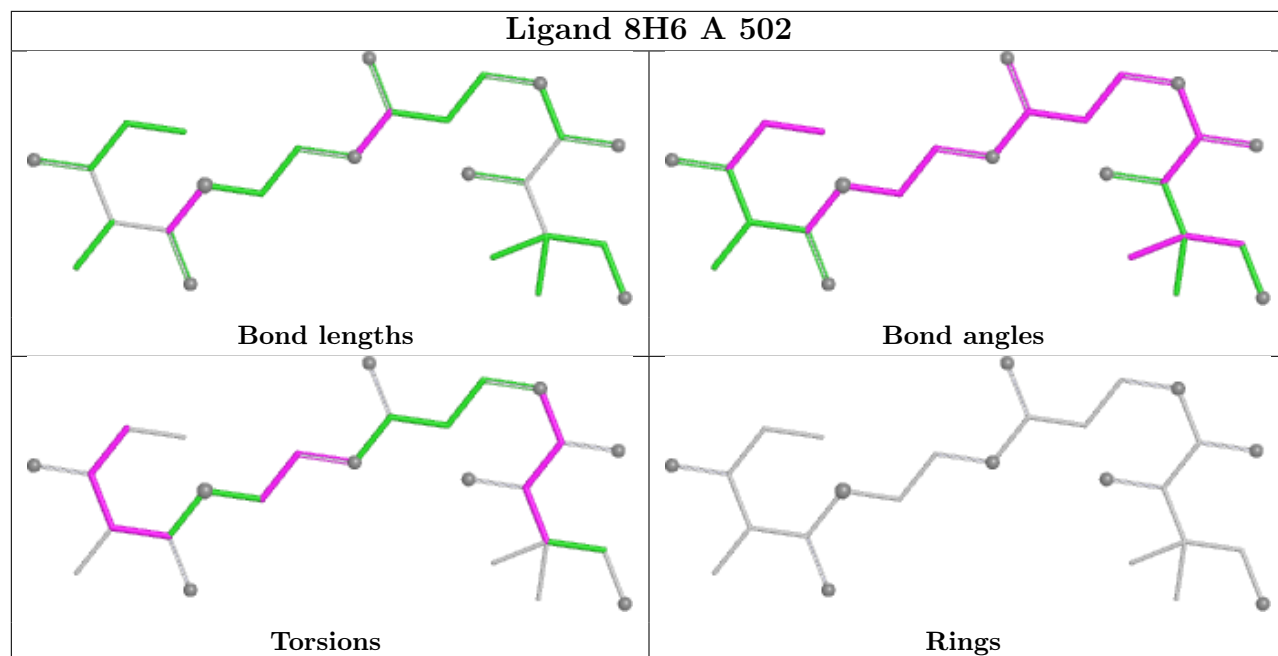
Mol	Chain	Res	Type	Atoms
3	B	502	8H6	C2-C3-C4-C5
3	B	502	8H6	C14-C3-C4-C5
3	B	502	8H6	C15-C3-C4-O16
3	B	502	8H6	C2-C3-C4-O16
3	B	502	8H6	C14-C3-C4-O16
3	B	502	8H6	C12-C11-N10-C9
3	B	502	8H6	N10-C11-C12-S13
3	B	502	8H6	S13-C19-C20-C26
3	B	502	8H6	C20-C21-C22-C23
3	B	502	8H6	O25-C21-C22-C23
2	A	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	C5D-O5D-PN-O1N
2	B	501	NDP	C5D-O5D-PN-O1N
2	A	501	NDP	PA-O3-PN-O2N
2	B	501	NDP	PA-O3-PN-O2N
3	A	502	8H6	S13-C19-C20-C26
3	A	502	8H6	C19-C20-C21-O25
2	A	501	NDP	PA-O3-PN-O1N
3	B	502	8H6	C20-C19-S13-C12
2	A	501	NDP	C3B-C2B-O2B-P2B
3	A	502	8H6	O16-C4-C5-N6

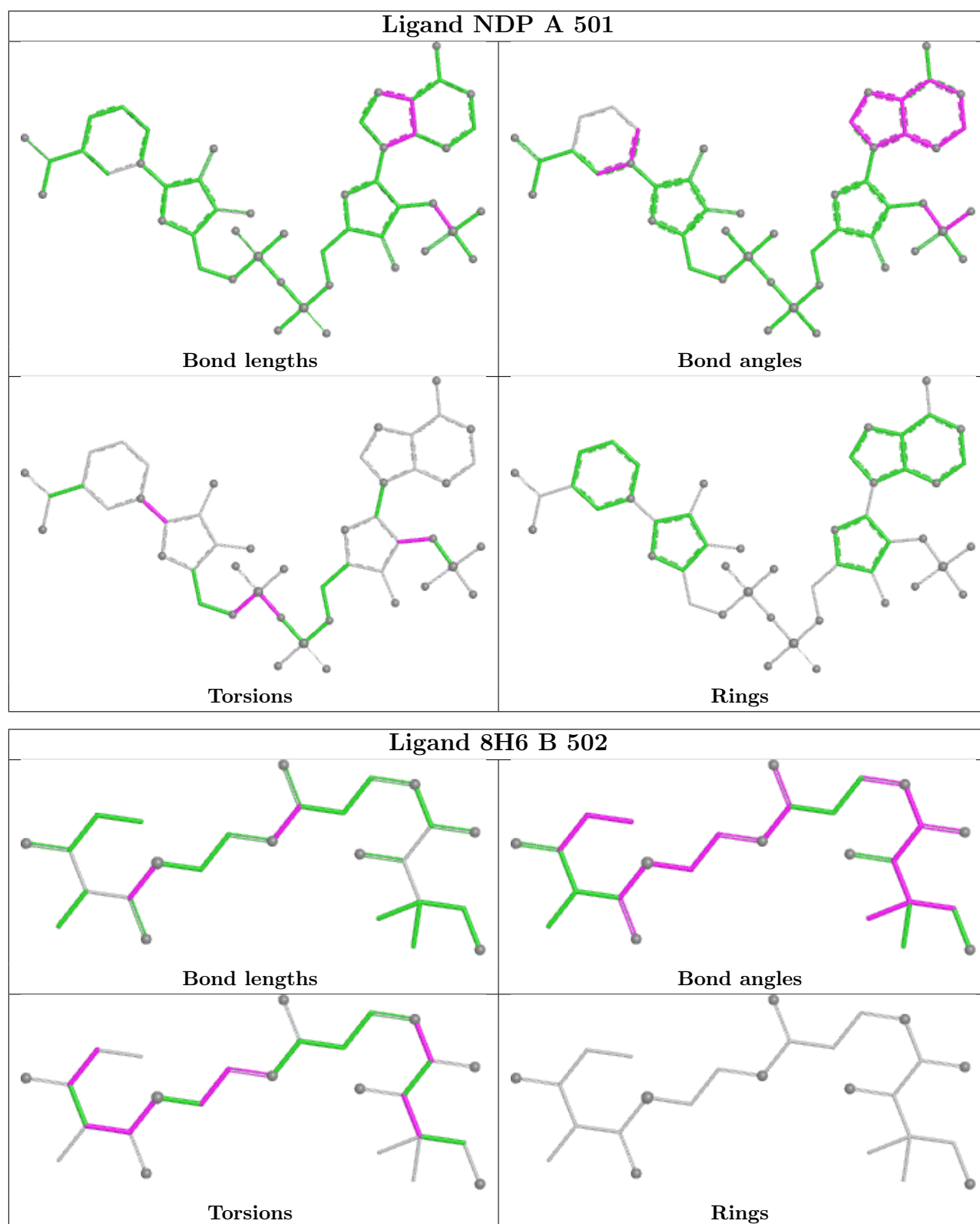
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	8H6	6	0
3	B	502	8H6	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	477/496 (96%)	0.76	52 (10%) 10 9	12, 21, 44, 66	0
1	B	477/496 (96%)	0.54	30 (6%) 26 24	11, 20, 41, 58	0
All	All	954/992 (96%)	0.65	82 (8%) 16 14	11, 21, 42, 66	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	5.4
1	A	210	GLY	5.0
1	A	407	VAL	4.9
1	A	209	PRO	4.5
1	A	208	VAL	4.4
1	A	213	LYS	3.8
1	B	211	SER	3.8
1	A	405	PRO	3.6
1	A	448	MET	3.5
1	B	19	ARG	3.3
1	A	130	GLY	3.3
1	A	410	ARG	3.2
1	A	131	ARG	3.2
1	A	211	SER	3.2
1	A	473	SER	3.2
1	A	229	GLY	3.1
1	B	-3	GLY	3.1
1	A	48	ASP	3.1
1	B	34	GLY	3.0
1	A	402	ALA	3.0
1	A	413	ARG	3.0
1	A	242	GLY	3.0
1	B	168	VAL	2.9
1	A	34	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	2.9
1	A	408	HIS	2.9
1	B	295	GLU	2.9
1	A	31	ASP	2.8
1	A	74	GLY	2.8
1	A	406	GLU	2.8
1	A	412	VAL	2.8
1	A	185	GLY	2.8
1	B	473	SER	2.7
1	A	71	GLU	2.7
1	B	268	GLN	2.7
1	A	91	THR	2.7
1	A	295	GLU	2.7
1	B	71	GLU	2.7
1	B	448	MET	2.7
1	A	115	LEU	2.7
1	A	89	LEU	2.6
1	A	296	ASP	2.6
1	A	409	ASP	2.6
1	B	91	THR	2.6
1	A	278	CYS	2.6
1	A	75	GLU	2.6
1	A	268	GLN	2.5
1	A	11	ARG	2.5
1	B	130	GLY	2.5
1	B	74	GLY	2.4
1	B	292	GLU	2.4
1	A	411	LEU	2.4
1	A	292	GLU	2.4
1	B	48	ASP	2.3
1	A	21	ALA	2.3
1	A	344	LEU	2.3
1	A	35	ALA	2.3
1	A	285	ALA	2.3
1	A	72	ASP	2.3
1	B	260	ALA	2.3
1	A	472	LEU	2.3
1	B	131	ARG	2.2
1	B	410	ARG	2.2
1	A	414	GLN	2.2
1	A	294	PRO	2.2
1	B	296	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	12	VAL	2.1
1	B	407	VAL	2.1
1	B	60	ALA	2.1
1	B	62	TRP	2.1
1	A	143	LEU	2.1
1	B	285	ALA	2.1
1	B	171	ARG	2.1
1	B	69	LEU	2.1
1	B	402	ALA	2.1
1	A	70	ARG	2.1
1	A	258	GLY	2.0
1	A	13	ALA	2.0
1	B	35	ALA	2.0
1	B	281	ALA	2.0
1	B	409	ASP	2.0
1	B	408	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

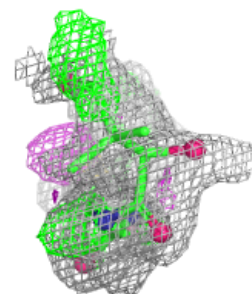
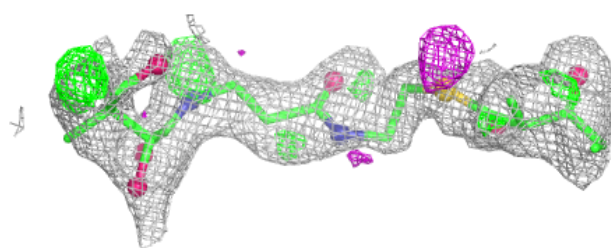
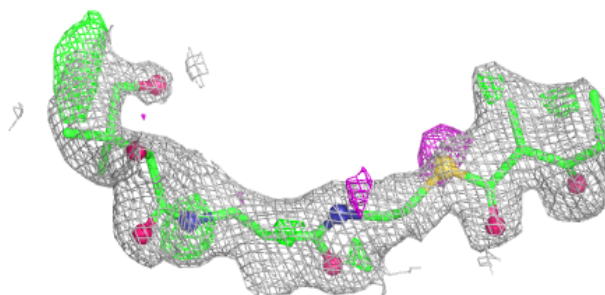
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	8H6	A	502	26/26	0.74	0.21	25,43,56,64	0
3	8H6	B	502	26/26	0.78	0.23	29,41,56,61	0
2	NDP	A	501	48/48	0.96	0.07	16,20,23,24	0
2	NDP	B	501	48/48	0.97	0.06	15,18,20,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

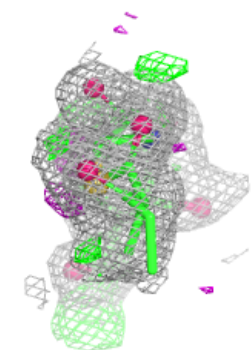
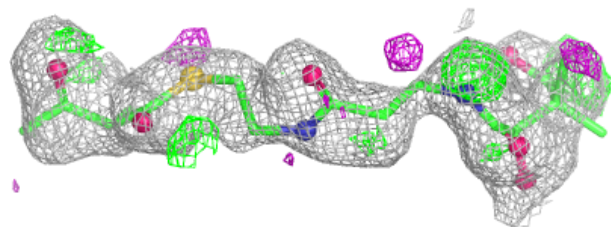
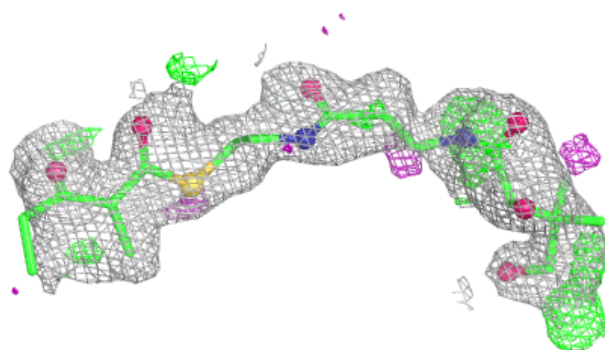
Electron density around 8H6 A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



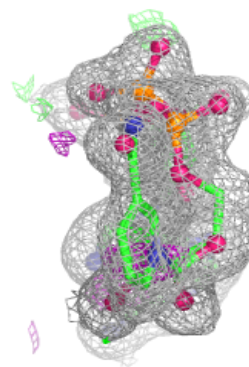
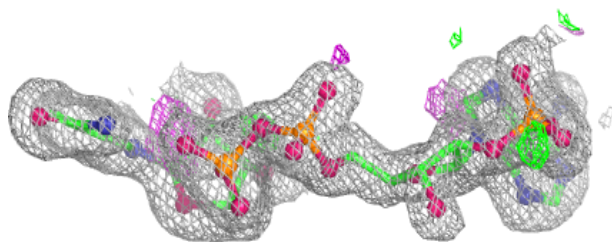
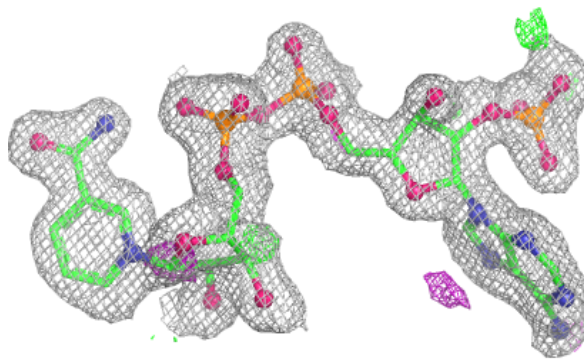
Electron density around 8H6 B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

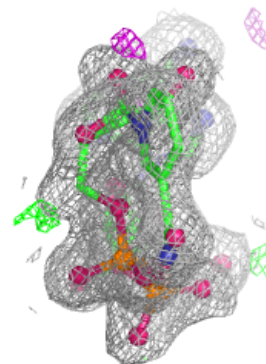
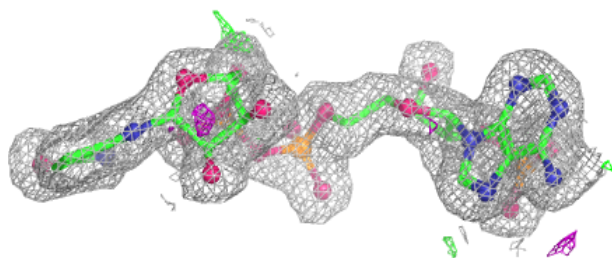
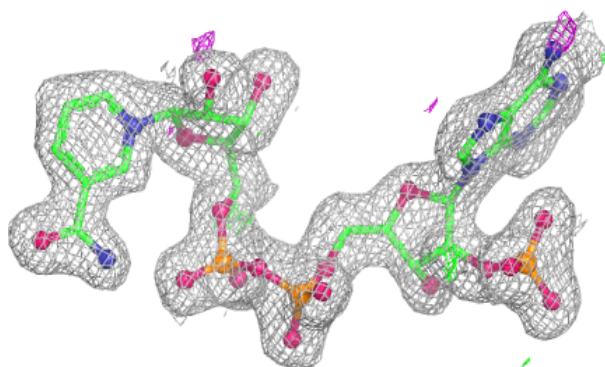


Electron density around NDP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NDP B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.